Total Credits= 23

2 nd Semester		Contact Hrs.			Marks		Credits	
Code	Name	L T P		Int.	Ext.	Total	Creuits	
MCHMS1-201	Molecular Spectroscopy-I	4	0	0	40	60	100	4
MCHMS1-202	Organometallics	4	0	0	40	60	100	4
MCHMS1-203	Organic Reactions & Mechanisms-II	4	0	0	40	60	100	4
MCHMS1-204	ACHMS1-204 Seminar - I 0 0 2		100		100	1		
Departmental Elective-II (Choose any one)								
MCHMD1-211	Nano Chemistry							
MCHMD1-212	Bio-organic Chemistry	4	0	0	40	60	100	4
MCHMD1-213	Analytical Chemistry							
Department	al Elective-III (Choose any one)							
MCHMD1-221	Natural Products							
MCHMD1-222	Bio-physical Chemistry	4	0	0	40	60	100	4
MCHMD1-223	Asymmetric Synthesis							
MCHMS1-205	Inorganic Chemistry LabII	0	0	4	60	40	100	2
	Total	20	0	06	360	340	700	23

MRSPTU M.Sc. CHEMISTRY SYLLABUS 2020 Batch

MOLECULAR SPECTROSCOPY-I						
Subject Code: MCHMS1-201 L T P C Duration: 60 (Hrs.)						
	4	0	0	4		

Course Objectives:

- 1. To introduce the concept of spectroscopy, selection rules, line width and broadening.
- 2. To familiarize with concepts of Microwave and Raman Spectroscopy
- 3. To provide the knowledge of concepts of Infrared and UV-visible Spectroscopy
- 4. To familiarize with concepts of NQR, Mossbauer and photoelectron Spectroscopy

Course Outcomes:

The students will acquire knowledge of

- 1. Selection rules, line width and broadening.
- 2. Various spectroscopic techniques.
- 3. Importance of spectroscopy for structural elucidation.

UNIT-I (15 Hours)

General Features of Spectroscopy

Introduction to spectroscopy, Nature of electromagnetic radiation, Regions of the electromagnetic spectrum Units and conversion factors, Intensities line width and line width broadening of spectral lines, transition probability, transition moment and selection rules

Microwave Spectroscopy

Classification of molecules according to their moment of inertia, Rotational spectra of rigid diatomic molecules, Intensities of spectral lines, isotopic substitution effects. Non-rigid rotator, Polyatomic molecules – Linear and symmetric top molecules, Stark effect

Raman Spectroscopy

Introduction, Classical and Quantam theory of Raman effect, Stokes and antistokes lines, anisotropic polarizability, Pure rotational raman spectra of linear and symmetric top molecules, vibrational raman spectra of H_2O and CO_2 molecules, Polarisation of the light and raman effect, Rule of mutual exclusion

UNIT-II (15 Hours)

Infrared Spectroscopy

Energy of vibrating diatomic molecule, simple harmonic oscillator, force constants, Fundamental vibration frequencies, Anharmonicity of molecular vibrations and its effect on vibrational frequencies, Frequencies of the vibrational transitions of HCl. Vibrational rotation spectra of CO, P, Q and R branches, Vibrations of polyatomic molecules. Examples of CO₂, H₂O, Mechanics of measurement of infrared and Raman spectra, absorption of common functional groups, their dependence onchemical environment (bond order, conjugation, H – bonding), Use of group theory to determine the number of active infrared and Raman active lines. Fermi resonance, combination bands and overtones, Infrared spectrometer, Application of IR in structure elucidation of organic compounds – Various Carbonyl compounds, alkane, alkenes, alkynes, unsubstituted, mono and di-substituted aromatic compounds, alcohols, phenols, ethers, Far IR region, Metal ligand vibrations, – CN, Nitronitrito- and CO ligands and the effect of their co-ordination with metal ions and IR spectra.

UNIT-III

UV and Visible Spectroscopy

Measurement technique, Beer – Lambert's Law, molar extinction coefficient, oscillator strength and intensity of the electronic transition, Frank Condon Principle, Ground and first excited electronic states of diatomic molecules, relationship of potential energy curves to electronic spectra. Chromophores, auxochromes, electronic spectra of polyatomic molecules, Woodward rules for conjugated dienes and α , β - unsaturated carbonyl groups, extended conjugated and aromatic sterically hindered systems, red shift, blue shift, hypo- and hyperchromic effect.

UNIT-IV

(16 Hours)

Mossbauer Spectroscopy

Mossbauer effect, Principles of Mossbauer spectroscopy, Formation of Mossbauer nuclides, Applications of Mossbauer spectroscopy

Photoelectron Spectroscopy

Introduction, Basic principles of electron spectroscopy, Photoelectric effect, Koopman's theorem, X-ray photoelectron spectroscopy (XPS) or ESCA, Instrumentation for XPS, chemical shifts in XPS, applications of XPS, ultraviolet photoelectron spectroscopy (UPS)

Nuclear Quadrupole Resonance

Introduction- quadrupole nuclei and quadrupole moment, experimental considerations, Electric Field Gradient (EFG), quadrupole coupling constant (QCC), Splitting in NQR spectra, Applications of NQR spectroscopy

Recommended Text Books / Reference Books:

- 1. Russell S. Drago, 'Physical Method for Chemistry', 2ndEdn., Surfside Scientific Publishers,**1992.**
- 2. R.M. Silverstein, G.C. Bassler, T.C. Morrill, 'Spectrometric Identification of Organic Compounds', 3rdEdn., Wiley, **1974**.
- 3. William Kemp, 'Organic Spectroscopy', 3rdEdn., W.H. Freeman, **1991**.
- 4. Dudley H. Williams & Ian Fleming, 'Spectroscopic Methods in Organic Chemistry', 6thEdn., McGraw Hill, Science,**2008.**
- 5. J.R. Dyer, 'Application of Absorption Spectroscopy of Organic Compounds', Prentice Hall, Englewood Cliffs, N.J., **1965**.
- Dudley H. Williams & Ian Fleming, 'Spectroscopic Problems in Organic Chemistry', 5thEdn., McGraw Hill, London, 1985.
- 7. R.C. Banks, E.R. Matjeka, G. Mercer, 'Introductory Problems in Spectroscopy' Manlo Park, CA, **1980**.
- 8. G.M. Barrow, 'Introduction to Molecular Spectroscopy', McGraw Hill, New York, **1962**.
- 9. C.N. Banwell 'Fundamentals of Molecular Spectroscopy' 4thEdn., TataMcGrawHill Education,**1994**.
- 10. D.L. Pavia, G.M. Lampan and G.S. Kriz, 'Introduction to Spectroscopy', 4thEdn., Cengage Learning, **2008**.
- 11. Jag Mohan, 'Organic Spectroscopy-principles and applications', 2ndEdn., Narosa Publishing house Pvt. Ltd., **2007**
- 12. P S Sindhu, 'Fundamentals of Molecular spectroscopy' 2ndEdn., New age international Publishers. **2011**

(14 Hours)

OR	GANOMETALLICS	
Subject Code: MCHMS1-202	L T P C	Duration: 60Hrs.
-	4004	

- 1. To recall classification of ligands and nomenclature of organometallic compounds.
- 2. To understand structure, bonding and reactivity of organometallic compounds.
- 3. To familiarize with the role of organometallic compounds in organic syntheses.
- 4. To understand the applications of organometallic compounds ascatalysts.

Course Outcomes:

The students will acquire knowledge of

- 1. Organometallic compounds and their nomenclature.
- 2. Bonding and reactivity of metal complexes.
- 3. Role of organometallic complexes in organic syntheses.
- 4. Importance of catalyst in syntheses.

UNIT-1 (11 Hrs.)

Introduction- Stability & decomposition pathways, classification of ligands, nomenclature of Organometallic compounds.

18 valence electron rule- Introduction to the 18 valence electron rule, total electron counts and finding metal-metal bonds & related problems.

UNIT-II (17 Hrs.)

Synthesis, structure, bonding & reactivity of organo transition metal complexes.

- a) Carbenes, Carbynes, Alkenes, Alkynes, Allylmoieties, Butadiene, Cyclobutadiene, Cyclopentadiene, Arenes, Cycloheptadienylmoieties & Cyclooctatetraenemoieties, Carbonyl.
- b) Ferrocenes- Structure & bonding of ferrocenes, basic chemical reactions of ferrocenes, chirality in ferrocene derivatives, ferrocene based condensation polymers.

UNIT-III (16 Hrs.)

Organometallic compounds in organic Synthesis-Green rules, synthesis & use of Zinc dialkyls, Collaman's reagent, organ mercuric& chromium carbonyls in organic synthesis, Heck reaction, Hydrozirconation.

UNIT-IV (16 Hrs.)

Applications of organometallic complexes to Catalysis-Basic principles, Industrial requirements of catalysts, sequences involved in catalytic reaction, asymmetric synthesis using catalyst, Hydrogenation catalysts & their classification, hydrogenation by lanthanide organometallic compounds. Hydro formylation: Cobalt catalyst & phosphine modified cobalt catalysts, Rhodium-phosphine catalysts, factors affecting n/iso ratio of hydro formylation products. Monsato, Cativa & Wacker processes, polymerization & oligomerisation of olefins & dienes, catalyticconverters.

Recommended Books

- 1. 'Basic Organometallic Chemistry: Concepts, Synthesis & Application of Transition Metals', CRC Press & Univ. Press, **2010**.
- 2. R.C. Mehrotra & A, Singh, 'Organometallic Chemistry, A Unified Approach', New Age International.
- 3. B.D. Gupta & A.J. Elias, 'Basic Organometallic Chemistry', UniversitiesPress.
 - 4. F.A. Cotton & G. Wilkinson, 'Advanced Inorg, Chemistry', WileyIntersciences.

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ORGANIC REACTION AND MECHANISM –II						
Subject Code:MCHMS1-203 L T P C Duration: 60 (Hrs.)						
	4	0	0	4		

Course Objectives:

- 1. To acquire the knowledge of addition to Carbon-Carbon and Carbon-Hetero Multiple Bonds
- 2. To understand the chemistry behind elimination, oxidation and reduction reactions.
- 3. To know the concepts of rearrangement reactions.
- 4. To acquire the knowledge and use of various reagents and retro synthetic approach used in organicsyntheses.

Course Outcomes:

The students will acquire knowledge of

- 1. Chemistry behind oxidation, reduction and Carbon-Carbon multiple bond reactions
- 2. Chemistry behind rearrangement reactions.
- 3. Use of diverse reagents in organicsynthesis
- 4. Retro synthetic approach in organic synthesis

UNIT-I (15 Hrs.)

1. Addition to Carbon-Carbon and Carbon-Hetero Multiple Bonds:

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation. Addition of Grignard reagents, organozinc, organolithium and Gillman reagents to carbonyl and unsaturated carbonyl compounds. Use of other organometallic reagents in addition reactions. Wittig reaction, Mechanism of condensation reactions involving enolates – Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

UNIT-II (15 Hrs.)

2. Oxidation :

Different oxidative processes. Hydrocarbons- alkenes, aromatic rings, saturated C-H groups) activated and inactivated). Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids. Amines, hydrazines, and sulphides.

Oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium (III) nitrate, DDQ, PCC, CAN, selenium dioxide, peroxyacids, DCC. Oxidation reactions with special emphasis on Baeyer-villeger reaction, Cannizarro oxidation-reduction reaction.

3. Reduction :

UNIT-III (15 Hrs.)

Different reductive processes, Hydrocarbons- alkanes, alkenes, alkynes and aromatic rings, Carbonyl compounds – aldehydes, ketones, acids, ester and nitriles. Epoxides, Nitro, nitroso, azo and oxime groups, Hydrogenolysis. Sodium borohydride, sodium cyano borohydride, LAH, disobutylaluminium hydride, tin hydride, trialkyl tin hydride, trialkylsilanes, alkoxy substituted LAH, DIBAL, diborane, diisoamyl borane, hexyl borane, 9-BBN, isopinocamphenyl and disiopinocamphenyl borane. Reduction reactions with particular emphasis on Wolf-Kishner reduction, Clemmensen reduction,

UNIT-IV (15 Hrs.)

4. Rearrangements :

General mechanistic consideration – nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements, Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Beckmann, Hofman, Curtius, Schmidt, Shapiro reaction, Fries rearrangement

5. Retrosynthesis:

Synthons and synthetic equivalents, Definitions, Guidelines, Functional group interconversions, Use of acetylenes and aliphatic nitrocompounds in organic synthesis; Two-group C-C disconnections – Diels-Alder reaction, 1,3- and 1,5-difunctional compounds (Michael addition and Robinson annulation), Order of events in organic synthesis, Chemoselectivity, Reversal of polarity (umpolung), Cyclisation reactions, Amine synthesis

Recommended Text Books / Reference Books:

- 1. Jerry March & Michael Smith, 'March's Advanced Organic Chemistry:Reactions, Mechanisms, and Structure', 6th Edn., John Wiley &Sons,2007.
- 2. Francis A. Carey & Richard J. Sundberg, 'Advanced Organic Chemistry: Structureand Mechanisms, Vol, A', 5th Edn., Springer,**2007**.
- 3. Francis A. Carey & Richard J. Sundberg, 'Advanced Organic Chemistry: Reactionand Synthesis', Vol. B, 4th Edn., Springer, **2006**.
- 4. K.C. Nicolaou and E.J. Sorensen, 'Classics in Total Synthesis: Targets, Strategies, Methods', Wiley, **1996**.

	SEMINAR – I	
Subject Code: MCHMS1-204	L T P C 0 0 2 1	Duration: 30 Hrs.

1. In the beginning of the semester, a teacher will be allocated maximum 30 students. The latter will guide/teach them how to prepare/present 15 minutes Power Point Presentation for the Seminar.

2. If there are more than 30 students in the class, then class will be divided into two group shaving equal students. Each group may be allocated to a different teacher.

3. Each student will be allotted a topic by the teacher at least one week in advance for the presentation. The topic for presentation may be from the syllabus or relevant to the syllabus of the program.

4. During the presentation being given by a student, all the other students of his/her group will attend the seminar. The assessment/evaluation will be done by the teacher. However, Head of Department and other faculty members may also attend the seminar, ask questions and give their suggestions.

5. This is a turn wise continuous process during the semester and a student will give minimum two presentations in a semester.

- 6. For the evaluation, the following criteria will be adopted,
- a) Attendance in seminar: 25 Marks
- b) Knowledge of subject along with Questions handling during the seminar: 25 Marks
- c) Presentation and communication Skills: 25 Marks
- d) Contents of the presentation: 25 Marks.

	NANOCHEMISTRY	
Subject Code: MCHMD1-211	L T PC	Duration: 60 Hrs.
	4004	

Course Objectives

- 1. To understand the concept of self-assembly and its applications to various nanostructures.
- 2. To understand synthesis of nanomaterials.
- 3. To learn characterization of nanomaterials.
- 4. To understand the applications of nano materials in biological system.

Course Outcomes:

The students will acquire knowledge of

- 1. Introduction to the concept of nanochemistry and its classification andterminology.
- 2. Synthesis of nanomaterials by different routes and their characterization. Applications in biological and electronic systems.

UNIT-I(15Hrs)

1. Introduction:

Introdution to nanochemistry and nanotechnology, definition & classification of nanomaterials. Properties & applications of nanomaterials.

2. Self-Assembly and Nanostructures:

Types of self-assemblies, self-assembling materials. Use of self-assembly in nano rod devices, nano wires, nano tubes, molecular logic gates, molecular storage devices, DNA, fullerenes, nano gas sensors.

UNIT-1I(15Hrs.)

3. Nano Material Synthesis:

Top down and bottom up approach, synthesis: Vapour phase synthesis by chemical routes; Nucleation & growth from solutions, stabilization against agglomeration. Processing of nano materials; Nano structured sol gel materials. Consolidation of nano crystalline materials by compaction and sintering, nanolithography.

UNIT-1II(15Hrs.)

4. Characterization Techniques:

Characterization of nano structured materials – by scattering techniques, proximal microscopy (AFM & STM).

UNIT-1V(15Hrs.)

5. Applications:

Bionano composites, biometrics, nano technology enabled sensors, Microelectronics,

drug delivery, bionano information.

Recommended Books:

- 1. C.P. Poole & F.J. Owens, 'Introduction to Nanotechnology', Wiley, 2003.
- 2. M. Ratner & D. Ratner, 'Nanotechnology', Prentice Hall, 2003.
- 3. M. Wilson, K. Kannagara, G. Smith, M. Simmons & B. Raguse 'Nanotechnology', CRC Press BocaRaton, 2002.
- 4. A. Ozin Geoffery & C. Andre, 'Nanochemistry, A Chemical Approach to Nanomaterials', Arsenault Royal Society of Chemists, **2005**.
- 5. E. Foster Lynn, 'Nanotechnology, Science Innovation & Opportunity', Pearsoneducation, 2007.

BIO-ORGANICCHEMISTRY							
Subject Code: MCHMD1-212	L T PC	Duration: 60 Hrs.					
	4004						

- 1. To illustrate the link between organic chemistry and biochemistry by discussing the organic chemistry of selected processes of living systems.
- 2. To integrate the chemical principles with biological applications with examples drawn from biochemistry, molecular and cellbiology.
- 3. To understand the mechanism of enzymecatalysis.
- 4. To understand the mechanism of combinatorial synthesis in medicinal chemistry.

Course Outcomes:

The students will acquire knowledge of

- 1. Relationship between organic chemistry and biochemistry.
- 2. Kinetics and mechanism of enzyme catalysis.
- 3. Determination of enantio- and diastereoselectivity using various analytical methods

UNIT-1 (15 Hrs.)

Amino Acids and Proteins:

Structure, classification, synthesis and properties of amino acids, isoelectric point, biosynthesis of amino acids. Peptides: oligo- and polypeptides, geometry of peptide linkage, N-terminal and C-terminal residue analysis, synthesis of peptides-amino and carboxyl protecting groups-solid phase peptide synthesis. Proteins: classification and properties (denaturation, isoelectric point and electrophoresis), primary, secondary, tertiary and quaternary structures of proteins, collagen and triple helix.

UNIT-1I (15 Hrs.)

Enzymes and Cofactors:

Mechanism of enzyme catalysis, Factors influencing enzyme action, Examples of typical enzyme mechanisms: chymotrypsin, ribonuclease and lysozyme, Enzyme-catalyzed addition, elimination, condensation, carboxylation and decarboxylation, isomerization, group transfer and rearrangement reactions-structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD+, NADP+, FMN, FAD, lipoic acid and Vitamin B12. Mechanisms of reactions catalyzed by the above cofactors.

UNIT-III (15 Hrs.)

Nucleic Acids and Protein Synthesis:

Nucleotides and nucleosides, DNA: primary and secondary structure-replication of DNA. RNA and protein synthesis: Messenger RNA synthesis-transcription, Ribosomes-rRNA, Transfer RNA, genetic code translation.

Determination of base sequence of DNA. Polymerase Chain Reaction (PCR). Antisense technology in chemotherapy and other nucleic acid-targeted drugs-intercalates, sequence specific drugs. A brief account of ribozyme and iRNA.

UNIT-IV (15 Hrs.)

Lead and Analogue Synthesis-1:

Designing organic synthesis-disconnection approach- synthons and synthetic equivalents-one group disconnections: alcohol, olefin, ketone, acids- two group disconnections: 1,2-, 1,3-, 1,4- and 1,5-difunctional compounds-convergent synthesis-functional group interconversions- functional group additions-carbon heteroatom bonds-methods for 3- to 6-membered rings.

Lead and Analogue Synthesis-2:

Combinatorial synthesis in medicinal chemistry: Solid phase techniques-methods of parallel synthesis-mix and split techniques-dynamic combinatorial chemistry-screening and deconvolution-limitations of combinatorial synthesis Asymmetric synthesis: basic principles-stereo selective and stereospecific reactions- methods for determining enantiomeric excess-chiral auxiliary, reagents and catalysts and their applications (wherever applicable) in alkylation, hydrogenation, hydroxylation, epoxidation and hydroboration of alkenes, reduction of ketones-Cram and Felkin-ahn models. Noyori's BINAP – Jacobson catalyst – Evans catalyst.

Recommended Books:

- 1. Hermann Dugas and C. Penny, 'Bioorganic Chemistry: A Chemical Approach to Enzyme action', Springer-Verlag.
- 2. N.C. Price and L. Stevens, 'Fundamentals of Enzymology', Oxford UniversityPress.
- 3. C. Walsh, W.H. Freeman, 'Enzymatic ReactionMechanisms'.
- 4. Stuart Warren, 'Designing Organic Synthesis: The Disconnection Approach', 2ndEdn., Wiley, **1984**.
- 5. H.B. Kagan, 'Asymmetric Synthesi', Thieme Medical Publishers, 2003.
- 6. Francis A. Carey and Richard B. Sundberg, 'Advanced Organic Chemistry: Part-A and Part-B', 5th Edn., Springer, **2007**.

ANALYTICAL CHEMISTRY

Subject Code: MCHMD1-213

L T P C 4 0 0 4 **Duration: 60 (Hrs.)**

Course Objectives:

- 1. To learn the theory and importance of analyticalchemistry.
- 2. To acquire knowledge about various methods of quantitative estimations.
- 3. To know the methods of analyzing the chemicals applying the electroanalytical and thermogravimetric instruments.
- 4. To know the methods of separating the mixture of compounds by chromatographic techniques.
- 5. To get familiar with various microscopic and radiochemical methods of analysis.

Course Outcomes:

The students will acquire knowledge of:

- 1. Basic concepts and importance of analytical chemistry.
- 2. Significance of significant figures and data analysis.
- 3. Thermogravimetric, electroanalytical, chromatographic and radiochemical methods of analysis.
- 4. Electron microscopic techniques and their application

UNIT-I (18 Hrs.)

Introduction to Analytical Chemistry

Classification of Analytical Methods. Types of samples, Preparation of sample for analysis, effect of sampling uncertainties, sample treatment, procedure of sampling of solids, liquids and gases.

Errors and Evaluation

Accuracy, precision, sensitivity, detection limits, significant figures, rounding off noise and sources, Uncertainties, errors. Types of errors – determinate and indeterminate errors. Ways of expressing accuracy, absolute and relative errors. Significant figures and propagation of errors. Confidence limit, Test of significance – the F-test and T-test. The statistical Q-test for rejection of a result, calibrations, mean, standard deviations. Linear least squares method. The correlation coefficient. Calculation for the above parameters.

Thermo analytical Techniques

Principle of thermogravimetry, thermogravimetric analysis, differential thermal analysis, differential scanning calorimetry, instrumentation for TGA, DTA and DSC, Methodology of TG, DTA and DSC. Application of TG to study of oxalates and chromates, factors affecting TGA and DTA curves. Applications of thermal analysis.

UNIT-II (15 Hrs.)

Electrochemical Techniques

a) D.C Polarography: Instrumentation - Dropping mercury electrode- -polarogram. Types of Currents: Residual, Migration, Limiting. Two and Three electrode assemblies. Ilkovic equation (derivation not required). Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants of complexes.

b) Brief account of following techniques:

(i) Pulse technique (ii) Differential pulse technique (iii) Cyclic Voltammetry (iv) Squarewave technique c) Amperometric titrations: Principle, Instrumentation. Types and applications amperometric titrations.

Chromatography

Classification of chromatographic techniques, differential migration rates, partition ratio, retention time, relation between partition ratio and retention time, capacity factor, selectivity factor. Efficiency of separation- resolution, diffusion, plate theory and rate theory HPLC: Principle, instrumentation, supports in HPLC. Applications of HPLC systems. Supercritical fluid chromatography (SFC). Recent developments in SFC and applications.

UNIT-III (12 Hrs.) Microscopy Techniques

Basic principle, instrumentation and applications of electron microscopy - SEM, TEM, scanning probe microscopy – STM, AFM.

Cryo-electron microscopy

Principle, instrumentation and applications, advantages and challenges, cryo-SEM, cryo-TEM, vitrification, cryo-electron microscopy of vitreous sections, ice contamination, cryo-negative staining, brief account of cryo-fixation methods, 2-D crystallization of membrane protein and cryo-preparation of 2-D crystal samples, brief discussion on cryo- electron tomography.

UNIT-IV (15 Hrs.)

Nuclear Chemistry:

Nuclear binding energy and stability, nuclear models (nuclear shell model and collective model). Nuclear reactions: types of reactions, nuclear cross-sections, Q-value. Natural and artificial radioactivity, radioactive decay and equilibrium, Nuclear fission-fission product and fission yields, Nuclear fusion.

Radiochemical methods of analysis:

Radioactive tracer techniques and its applications, isotope dilution analysis, neutron activation analysis, Counting techniques such as G.M. Ionization and proportional counters.

Separation methods:

Solvent extraction: Partition law and its limitations, distribution ation, separation factor, factor influencing extraction, multiple extractions.

Recommended Text Books / Reference Books:

- 1. A Douglas, Skoog and Donald M. West, F.J. Holler, 'Fundamentals of Analytical Chemistry', 8thEdn., Harcourt College Publishers, **2004**.
- 2. Skoog, Holder, Nieman, 'Principles of Instrumental Analysis', 5thEdn., Thomson Books, **1998**.
- 3. J. Mendham, R.C. Denney, J.D. Barnes, M. Thomas, 'Vogel's Text Book of Quantitative Chemical Analysis', 6thEdn., Pearson Education, **2006**.
- 4. R. Gopalan, P.S. Subramaniam and K. Rengarajan, 'Elements of Analytical Chemistry', 3rdEdn.,Sultan Chand and Sons,**2003**.
- 5. S. Usharani, 'Analytical Chemistry', Macmillan Publishers, 2000.
- 6. A. Cavalier, D. Spehner, B.M. Humbel, 'Handbook of Cryo-Preparation Methods for Electron Microscopy', CRC Press, Taylor & Francis Group, **2009**.
- 7. B. C. Harvey, 'Introduction to Nuclear Chemistry', Prentice-Hall, 1969.
- 8. G. Friedlander, J. W. Kennedy, E.S. Marcus, J.M. Miller, 'Nuclear & Radiochemistry', John Wiley & Sons, **1981**.

 H.J. Arnikar, 'Nuclear Chemistry', Wiley Eastern Co., II Edition, 1987.
A. Braithwaite and F.J. Smith, 'Chromatographic Methods',5th Ed., Blackie Academic and Professional, London, 1996.

		NATURAL PRODUCTS	
Subject Cod	e: MCHMD1-221	L T PC 4004	Duration: 60Hrs.

- 1. To acquire basic knowledge of isolation, purification, identification and standardization of natural products.
- 2. To discuss structure elucidation of alkaloids and terpenoids.
- 3. To discuss isolation, purification and structure elucidation of sterols
- 4. To understand the importance of vitamins, xanthophyll and carotenes.

Course Outcomes:

The students will acquire knowledge of

- 1. Isolation, purification, identification and standardization of natural products.
- 2. Structure elucidation of alkaloids, sterols and terpenoids,
- 3. Importance of vitamins, xanthophyll and carotenes.

UNIT-I (15 Hrs.)

1. Introduction & General Methods

Isolation, purification, identification and standardization of natural products. Carbohydrates and metabolism: Introduction, stereoisomerism, mutarotation, configuration and ring structure of monosaccharides, disaccharides and polysaccharides. Glycolysis, alcoholic and lactic acid fermentation, citric acid cycle.

UNIT-II (15 Hrs.)

Introduction, classification, isolation and purification of alkaloids and terpenoids. Structure elucidation of alkaloids (atropine, quinine, morphine) and terpenoids (camphor and menthol). Biosynthesis of alkaloids and terpenoids.

UNIT-III (15Hrs.)

2. Steroids

General introduction, isolation, purification and structure elucidation stereochemistry of sterols with special reference to cholesterol. Vitamin D group and bile acids. Biosynthesis of sterols.

UNIT-IV (15Hrs.)

3. Carotenoids and Vitamins

Introduction to carotenoids and vitamins, Carotenes. Vitamin A, xanthophyll, vitamin B complex, vitamin K and vitamin E group.

Recommended Books

- 1. I.L. Finar, 'Organic Chemistry: Stereochemistry and The Chemistry Natural Products', Vol. II, 5th Edn., Longman Scientific & Technical, **1988**.
- 2. O.P. Agarwal, 'Chemistry of Organic Natural Products', Vol. I, 40thEdn., Krishna Prakashan Media,2010.
- **3.** O.P. Aggarwal, 'Organic Chemistry Natural Products', Vol. II, 38th Edn.,Krishna Prakashan Media,**2010.**

BIO-PHYSICALCHEMISTRY							
Subject Code: MCHMD1-222	L T PC	Duration: 60Hrs.					
	4004						

- 1. To equip with basic knowledge of the physical principles that governs chemical systems.
- 2. To provide knowledge of various biological systems with emphasis onbiochemical reactions.
- 3. To recall enzymes, their role in chemical and biological catalysis.
- 4. To understand various principles that govern cellularprocesses.

Course Outcomes:

The students will acquire knowledge of

- 1. Basic concepts and mechanism of enzyme catalyzedreactions.
- 2. Interactions between various biomolecules.
- 3. Thermodynamics of ADP and ATP syntheses

UNIT I (15Hrs)

Biological Cell and its Constituents:

Biological cell, DNA and RNA in living systems. Basic consideration. Proximity effects and molecular adaptation.

Enzymes:

Introduction and historical perspective, chemical and biological catalysis, Remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis-Menten and Line Weaver-Burk plots, reversible and irreversible inhibition.

UNIT II (15Hrs)

Kinds of Reactions Catalyzed by Enzymes:

Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reaction, enolic intermediates in isomerization reactions, b-cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

Co-Enzyme Chemistry:

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological function of coenzyme A, thiamine pyrophosphate, Pyridoxal phosphate, NAD+, NADP+, FMN, FAD, lipoic acid, vitamin B12. Mechanism of reaction catalyzed by the above cofactors.

UNIT III (15Hrs)

Biological Macromolecules: The Nucleic Acids:

Nucleotide, torsion angles in poly nucleotide chains, the helical structure of polynucleic acids, high order structure in polynucleotides.

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Interactions in Macromolecules:

Basic principles of interaction between molecules, water structure and its interaction with biomolecules, dipole interactions, side chain interactions, electrostatic interactions, base pairing in nucleic acids, base stacking, hydration and the hydrophobic effect.

Structural Transition in Bio-macromolecules:

Coil – helix transitions in proteins, statistical methods for predicting protein secondary structures; melting and annealing of polynucleotide duplexes, helical transitions in double stranded DNA, super coil dependent DNA transitions predicting helical structures in genomic DNA.

UNIT IV (15 Hrs)

Bioenergetics and ATP cycle

Standard free energy change in biochemical reaction, exergonic, endergonic reactions. Hydrolysis of ATP, synthesis of ATP from ADP, metal complexes and transition of energy, chlorophylls, photo system I and photo system II in cleavage of water.

Thermodynamics of Biopolymer Solutions

Thermodynamics of biopolymers solutions, osmotic pressure, membrane equilibrium, muscular contraction and Energy generations in mechano-chemical system.

Recommended Books:

- 1. A.L. Lehninger, 'Principles of Biochemistry', WorthPublishers.
- 2. Voet; 'VoetBiochemistry', John Wiley, 1995.
- 3. E.E. Conn, P.K. Stumpt, 'Outlines of Biochemistry', JohnWiley.
- 4. Hermann Dugas, C. Penny, 'Bioorganic Chemistry: Chemical Approach toEnzyme Action', Springer Verlag, **1982**.
- 5. M.I. Page, A. Williams, 'Enzyme Mechanisms, 'Royal Society of Chemistry'.
- 6. Richard B. Silverman, 'Organic Chemistry of Enzyme CatalysedReaction'.
- 7. I. Bertini, H.B. Gray, S.J. Lippard, J.S. Valentine, 'Bioinorganic <u>Chemistry'</u>, UniversityScience Books.
- 8. William Jolley, 'BioinorganicChemistry'.
- 9. K.E. VanHolde, W.C. Johnson, P.S. Ho, 'Principles of Physical Biochemistry', Prentice Hall, **1998**.
- 10. L.Stryer, 'Biochemistry', W.H.Freeman.
- 11. J. DavidRawn, 'Biochemistry', NeilPatterson.
- 12. F. Wold, 'Macromolecules: Structure and Function', PrenticeHall.
- 13. C.R. Cantor, P.R. Schimmel, 'Biophysical Chemistry', Vol. 1-3, Freeman, 1980.

ASYMMETRIC SYNTHESIS

Subject Code: MCHMD1-223

L T P C 4 0 0 4 **Duration: 60 (Hrs.)**

Course Objectives:

- 1. To learn the theory and importance of asymmetric Synthesis.
- 2. To acquire knowledge of various concepts of inducing enantio- and diastereoselectivity.
- 3. To give an understanding of various methods of asymmetric Synthesis.
- 4. To understand various analytical methods used for purifications & separations.

Course Outcomes:

The students will acquire knowledge of:

- 1. Methods for inducing enantio- and diastereoselectivity.
- 2. Determination of enantio- and diastereoselectivity using various analyticalmethods.
- 3. Chemistry behind a range of asymmetric reactions

UNIT-I (18 Hrs.)

Basic Principles of Chirality and Asymmetric Synthesis:

Phenomenon of chirality, Need for asymmetric synthesis, Selective synthesis of enantiomers, Enantiomeric purity of natural products, stereogenic unit and types of chiral compound, Centrally chiral compounds of carbon, Centrally chiral compounds of nitrogen and phosphorus, Centrally chiral compounds of sulphur, Axially chiral compounds, Chiral molecules with more than one stereo genic unit: diastereomers, The selective synthesis of diastereomers, Prochirality: enantotopic and diastereotopic groups. Definition: enantiotropic and diastereotropic groups and faces – Symmetry, substitution and addition criteria. Prochirality nomenclature: Pro – R, Pro – S, Re and Si. Selectivity in synthesis: Stereospecific reactions (substrate stereoselectivity), Stereoselective reaction (Product stereoselectivity), Enantioselectivity and diastereoselectivity. Chemoselectivity, Regioselectivity. Conditions of Stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods for inducing enantio- and diastereoselectivity.

UNIT-II (12 Hrs.)

Analytical Methods:

Determining % Enantiomeric excess, % Enantioselctivity, Optical Purity, % Diastereomeric excess and % diatereoselectivity. Resolving agents and resolution of recemic compounds having common functional groups e.g. alcohol, amine, acid. Techniques for determination of Enantioselectivity, Polarimetric methods, Gas chromatography methods, Liquid chromatographic methods. NMR spectroscopy-Chiral derivatising agents (CDAs), Chiral solvating agents (CSAs), Chiral lanthanide shift reagents (CLSRs).

UNIT-III (18 Hrs.)

Classification of Asymmetric Reactions:

- i) Substrate controlled asymmetric synthesis: Nucleophilic addition to chiral carbonyl compounds, 1,2 –Asymmetric induction, Felkin-Anh model, Double stereo differentiation; matched pair and mismatched pair, Examples from aldol condensation and hydroborationreactions
- ii) Chiral auxiliary controlled asymmetric synthesis: α-alkylation of chiral enolates, azaenolates, imines and hydrazones, chiral sulphoxides. 1,4-asymmetric induction and Prelog's rule, use of chiral auxiliary in Diels-Alder and Cope reactions
- iii) Chiral reagent controlled asymmetric synthesis: Asymmetric reduction using BINAL-H. Asymmetric Michael addition to α , β -unsaturated carbonyl compounds, Chiral lithium amides- enantioselective deprotonation, applications of chiralorganoboranes.

UNIT-IV (12 Hrs.)

Classification of Asymmetric Reactions (Continued Unit III):

iv) Chiral catalyst controlled asymmetric synthesis: Sharpless, Jacobson and Shi

asymmetric epoxidation, Sharpless asymmetric dihydroxylation and amino hydroxylation. Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalyst. Chiral catalyst controlled Diels-Alder and Michael reactions, Jacobson Catalysts-Evans Catalyst- Aziridination, Enzyme mediated enantioselective synthesis.

Recommended Text Books / Reference Books:

- 1. R. A. Aitken, S. N. Kilenyi, Asymmetric Synthesis, Originally published by Chapman &Hall, **1992**.
- 2. Guo-Qiang Lin, Yue-Ming Li, Albert S. C. Chan, Princilpes and applications of Asymmetric Synthesis, Wiley Interscience, **2001**
- 3. J.D. Morrison and H.S. Moscher, 'Asymmetric Organic Reactions', Vol 1-5, Academic Press, **1983.**
- 4. E.N. Jacobsen, A. Pfaltz, H. Yamamoto, 'Comprehensive Asymmetric Catalysis', Eds. Springer, **2000.**
- 5. R.S. Ward, 'Stereoselectivity in Organic Molecules', Wiley, New York, 1999.
- 6. E.L. Eliel, 'Stereochemistry of Carbon Compounds', Wiley, 1992.
- 7. W. Carruthers, 'Some Modern Methods of Organic Synthesis', Cambridge University Press, 4th Edn.,**2012.**
- 8. I. Ojima, 'Catalytic Asymmetric Synthesis', VCH-NY, Pergamon. 1998.
- 9. R.E. Gawley, J. Aube, 'Principles of Asymmetric Synthesis' (Tetrahedron Series in Organic Chemistry), Pergamon, **1996.**
- 10. H.B. Kagan, 'Asymmetric Synthesis', Edn., I, Thieme Medical Publishers, 2003.
- 11. G. Proctor, 'Asymmetric Synthesis', Oxford University Press, USA, 1997.

INORGANIC CHEMISTRY LAB-II							
Subject Code: MCHMS1-205	L T P C 0 0 4 2	Duration – 60 Hrs.					

- 1. To extend knowledge of use of standard laboratory equipment, modern instrumentation and classical techniques to carry out experiments.
- 2. To synthesize various inorganic complexes and their qualitative determination by UV,IR, NMR and ESR techniques.

Course Outcomes:

The students will acquire knowledge of

- 1. Volumetric and gravimetric analysis of cations and anions.
- 2. Understand electro analytical techniques.
- 3. Syntheses of various complexes and their structural analysis.
- 4. Use of various spectroscopic techniques like UV, IR, NMR for structural determination. **Note:**
- 1. Students will have to perform atleast 10-12 experiments from the given syllabus.
- 2. Any other subject related experiment can also be included.
 - **1. Gravimetric Analysis of Cations and Anions:** Iodide, thiocyanate, Sulphate, oxalate chloride, nickel, copper cobalt, zinc and their mixture.

2. Determination of Metal Ions Using Solvent Extraction:

- a) Determination of copper as the diethydithiocarbamatecomplex
- b) Determination of iron as the 8hydroxyquinolate
- c) Determination of nickel as the dimethylglyoxime complex,
- **3. Electro Analytical Techniques** pHmetric, Conductometric Titration: Representative acid/base and redox titrations.
- 4. Colorimetry and Spectrophotometry
 - a) Determination of λ_{max} the absorption curve and concentration of asubstance
 - b) Determination of copper (II) with EDTA
 - c) Determination of iron (III) with EDTA.

Recommended Books:

- 1. H. Denny, W. Roesky, 'Chemical Curiosites', WILEY VCH,1996.
- 2. G. Marr and B.W. Rocket, 'Practical Inorganic Chemistry', University ScienceBooks, 1999.
- 3. G. Pass and H. Sutcliffe, 'Practical Inorganic Chemistry', Chapman and Hall,London, 1968.
- 4. J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, 'Vogel's Textbook of Quantitative Analysis', Pearson Education, **2006**.
- 5. G. Svehla, 'Vogel's Textbook of Quantitative Analysis', PearsonEducation, 2006.
- 6. Anil J. Elias, 'A Collection of Interesting General Chemistry Experiments', University Press, **2002**.

Note: The students are required to perform atleast 2 experiments from each section.